

HERMESv3_GR: A stand-alone multiscale emission processing system

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1. INTRODUCTION

Emission inputs of trace gases and aerosols play a key role in the performance of Chemical Transport Models (CTMs). New and updated global and regional emission inventories are continuously being developed and made publicly available by research groups and international programs. Nevertheless, the reporting format of these inventories is usually not compatible with the emission input requirements of CTMs (i.e. hourly and chemical species-based emissions distributed over specific grid projections and resolutions, and using specific file formats and conventions). We describe the High-Effective Resolution Modelling Emission System version 3 – Global_Regional (HERMESv3_GR), a highly customizable emission processing system that calculates emissions from different sources, regions and pollutants over a user-specified global or regional model grid and fulfills the requirements of several CTMs.

2. MODEL DESCRIPTION

A general representation of the HERMESv3_GR workflow is provided in Figure 1. The user can flexibly define combinations of existing global and regional emission inventories, and apply regional scaling factors and masks. Each inventory is processed using vertical, temporal and speciation profiles that are also defined by the user. The definition of the working domain accepts several map projections (i.e. equirectangular, rotated pole, lambert conformal conic, mercator). The selection of emission inventories and databases is done through detailed configuration files, which provides the user with a widely applicable framework for designing, choosing and adjusting the emission modelling experiment without changing any source code. The outputs of HERMESv3_GR have been tested in several CTMs, including CMAQ, WRF-Chem and NMMB-MONARCH.

The emission calculation process implemented within HERMESv3_GR consists of

five steps: (i) spatial regridding from source grid to destination grid, (ii) vertical distribution, (iii) temporal disaggregation, (iv) speciation mapping to the selected gas phase and aerosol chemical mechanisms and (v) writing of the output following the nomenclature of the selected CTM.

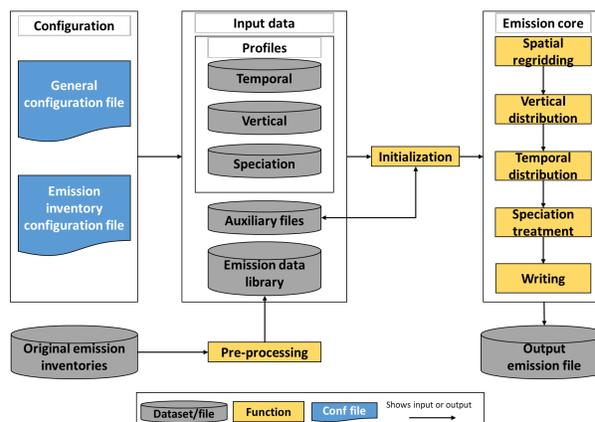


Fig. 1. Representation of the general structure of HERMESv3_GR

2.2 Emission data library

HERMESv3_GR can process most of the current state-of-the-art available emission inventories.

At the global scale, the available datasets include the Air Pollutants and Greenhouse Gases Emission Database for Global Atmospheric Research (EDGAR v4.3.2_AP, Cripa et al., 2018, EDGARv4.3.2_VOC, Huang et al., 2017), the Community Emissions Data System (CEDS, Hoesly et al. 2018) as well as the inventories derived from the Task Force Hemispheric Transport of Air Pollution community (HTAPv2.2, Janssens-Maenhout et al., 2015) and the Evaluating the Climate and Air Quality Impacts of Short-Lived Pollutants project (ECLIPSEv5.a, Klimont et al., 2017). Also at the global scale, biomass burning emissions are provided by the Global Fire Assimilation System (GFASv1.2, Kaiser et al. 2012), whereas open burning of

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domestic waste and volcanic degassing emissions can be estimated using the inventories reported by Wiedinmyer et al. (2014) and Carn et al. (2017), respectively. Two regional anthropogenic emission inventories are also included, namely the TNO-MACC_III (Kuenen et al., 2014) and the EMEP (Mareckova et al., 2017).

Natural emissions such as biogenic NMVOCs, mineral dust aerosols, Ocean DMS or lightning NO, which have functional dependencies on meteorological variables, are assumed to be calculated online during the execution of the corresponding CTM.

2.3 Emission inventory configuration file

The emission inventory configuration file allows selecting the emission inventories, pollutant sectors and species that will be combined. For each emission inventory/pollutant specie(s) the user can define:

- Country-specific scaling factors that multiply the original emissions.
- Country-specific masks that restrict the applicability of the original inventory to a given region.
- A vertical profile to distribute the original emissions across the vertical layers of the working domain.
- A monthly, daily and hourly profile to temporally disaggregate the original emissions.
- A speciation profile to map the original pollutants species to a specific gas phase and aerosol chemical mechanism.

Figure 2 shows five examples of the outputs that can be obtained depending on the definition of the emission inventory configuration file. In the first example (top-left), the user is selecting the 2010 HTAPv2.2 organic carbon (OC) transport emissions, while in the second one (top-right) this inventory is combined with the OC biomass burning emissions estimated by GFASv1.2. The third example (mid-left) illustrates how the original HTAPv2.2 OC transport emissions are being scaled by a factor of 5 in China and 0.5 in India. In the fourth example (mid-right), the user is masking out the emissions reported in China and India, while in the last example (bottom-centred) the OC transport emissions reported by ECLIPSEv5a in China and India and being combined with HTAPv2.2.

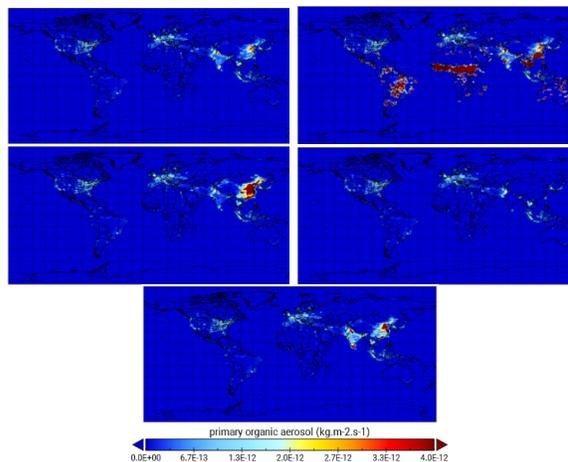


Fig. 2. Examples of organic carbon global emission outputs obtained with HERMESv3_GR using different versions of the emission inventory configuration file.

2.4 Spatial regridding

This function regrids the selected inventories from their original source grid to the user-defined destination grid. The regridding process is broken into two steps. The first step uses the Earth System Modeling Framework (ESMF) regrid weight generation application (Hill et al., 2004) to calculate an interpolation weight matrix that describes how points in the source grid contribute to points in the destination grid. The interpolation method used is a first-order conservative option, which performs the weight calculation based on the ratio of source cell area overlapped with the corresponding destination cell area. The second step is the multiplication of emissions on the source grid by the interpolation weight matrix and, if previously defined by the user in the emission inventory configuration file, the corresponding scaling and/or masking factors to produce emissions on the destination grid. Country-specific scaling and masking factors are generated using as a basis a gridded country mask created during the initialization process.

The regridding process allows the user to interpolate the original emissions to global or regional grids with flexible spatial resolutions and several map projections, including Equirectangular, Rotated pole, Lambert conformal conic and Mercator (Figure 3).

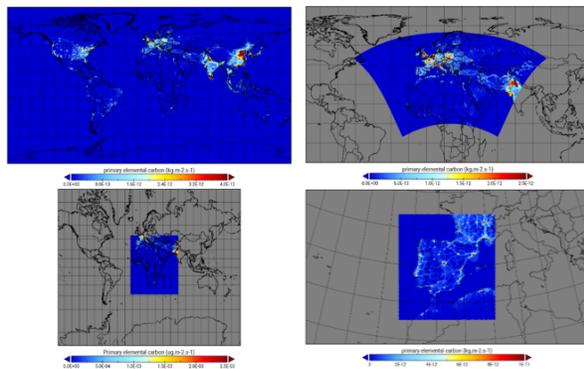


Fig. 3. Examples of the HTAPv2.2 black carbon transport emissions interpolated to a: 1*1.4deg global regular lat-lon domain (top-left), 0.1*0.1deg rotated lat-lon domain (top-right), 50kmx50km mercator grid (bottom-left) and 4kmx4km lambert conformal conic grid (bottom-right)

2.5 Vertical distribution

Once the model has horizontally allocated the total emissions, the next step consists of vertically distributing them across the vertical layers of the destination modelling domain.

The user is able to define and assign any fixed vertical profile to any emission inventory/pollutant sector/pollutant specie(s). Some suggested vertical profiles for the energy and manufacturing industry (Bieser et al., 2011) and the air traffic sectors (Olsen et al., 2013) are included in the HERMESv3_GR profiles database.

2.6 Temporal distribution

This process distributes temporally the emissions from their original resolution (e.g. annual) to the one defined by the user (monthly, daily or hourly). The emissions are multiplied by the user-defined monthly, weekly and hourly weight factors, which can be supplied as fixed profiles or using gridded files, which contain specific weight factors for each grid cell. The application of gridded profiles can be of importance for those emission sectors whose temporal variation is not uniform across the space due to local influences such as temperature (e.g. residential combustion emissions) or farming practices (e.g. agricultural emissions). As in the case of the vertical profiles, the user is left free to define and assign any temporal profile to each pollutant sector and specie. The HERMESv3_GR profiles database includes by default the monthly, daily and hourly temporal profiles reported by

LOTOS-EUROS (Denier van der Gon et al., 2011), which are partially based on the GENEMIS project (Friedrich and Reiss, 2004). The hourly temporal profile proposed by Hodzic et al (2012) for distributing trash burning emissions are also included.

2.7 Speciation mapping

During this process the model performs a mapping of the pollutants provided in the original emission inventories to the species needed by the CTM of interest and corresponding chemical mechanism. The HERMESv3_GR database includes speciation profiles for the Carbon Bond 05 (CB05), Carbon Bond 05 e51 (CB05e51) and the Regional Acid Deposition Model 2nd generation (RADM2) gas-phase and the fifth/sixth-generation aerosol module (AERO5, AERO6) and the Modal Aerosol Dynamics Model for Europe with the secondary organic aerosol model (MADE/SORGAM) aerosol mechanisms. For NMVOCs, most of the proposed speciation profiles are based on the availability of mapping tables described in Carter (2015). In the case of PM2.5, mappings are mostly based on the SPECIATE (Simon et al., 2010) and SPECIEUROPE (Pernigotti et al., 2016) databases and the works by Visschedijk et al. (2007) and Reff et al. (2009). As in the case of the temporal and vertical weight factors, the user is able to create its own speciation profiles using other sources of information.

2.8 Technical implementation

HERMESv3_GR is coded using Python 2.7.X and requires numpy, netCDF4, cdo, pandas, geopandas, pyproj, configargparse, cf_units, ESMPy, holidays, pytz, timezonefinder and mpi4py Python libraries.

The emission core module of HERMESv3_GR is parallelized using a map partitioning strategy (Figure 4). During the spatial regridding, the destination working domain is divided into vertical sections, maintaining each column undividable. The number of divisions is equal to the number of processors to be used (P_0, P_1, ...), which is defined by the user. The 2D regridded emissions are kept in memory until the writing operation. During this task, the vertical (v0, v1, ...) and temporal (t0, t1, ...) weight factors previously estimated in the vertical and temporal distribution functions are applied to each emission subdomain in order to transform the 2D arrays (longitude, latitude) into 4D arrays (time, vertical layer,

longitude, latitude). Finally, each worker process writes simultaneously its result to a common NetCDF4 file, which ensures the gathering of the different subsets of the working domain into a single output.

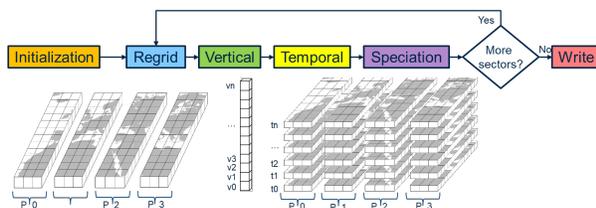


Fig. 4. Schematic representation of the parallelization of the emission core module of HERMESv3_GR

3. APPLICATIONS

HERMESv3-GR is currently implemented in two forecasting systems, namely in the NMMB-MONARCH model that participated in the International Cooperative for Aerosol Prediction (ICAP) multi-model ensemble (www.nrlmry.navy.mil/aerosol/icap.1135.php) and the AIRE-CDMX air quality forecasting system for Mexico City (<http://www.aire.cdmx.gob.mx/pronostico-aire/>). HERMESv3_GR has been also used to perform simulations with the CALIOPE air quality system (<http://www.bsc.es/caliope/en/forecasts?language=en>) and in several tests using WRF-Chem.

4. CONCLUSIONS

HERMESv3_GR is designed to provide a flexible and simplified framework for the generation of emission input files for global and regional air quality modelling. The main advantages of the model are as follows:

- User-defined grid and choice between different map projections: global or regional domain with a equirectangular, rotated pole, mercator or lambert conformal conic projection.
- Choice and combination of different emission inventories: the emission data library of HERMESv3_GR includes current state-of-the-art global and regional inventories that cover different sources (anthropogenic, biomass burning, volcanoes), pollutants (ozone precursor gases, acidifying gases and primary particulates) and base years (past, present and future).

- Choice between different vertical, temporal and speciation profiles.
- Choice between different CTMs: output files can be used as input for CMAQ, WRF-CHEM and NMMB-MONARCH.
- Choice between different chemical mechanisms: base pollutants can be mapped to the CB05, CB05e51, RADM2, AERO5, AERO6 and MADE/SORGAM mechanisms.
- Parallel implementation: The emission core module of HERMESv3_GR is parallelized, which allows decreasing the execution time and memory consumption of the model. This feature can be of importance when using the model in operational air quality forecasting systems.

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